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Multi-level deformation of thin films caused by stress-strain distribution at the film-substrate interface

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Abstract

The processes of elastic deformation of thin films on substrates under thermal and mechanical loadings were investigated. Mechanisms of formation of wrinkle and buckle patterns on the surfaces of metal and oxide films are studied. It is demonstrated that important role is played by the periodical distribution of stresses and strains at the film-substrate interface underlying the deformation of thin films subjected to different external loadings.

Keywords: Thin films; stresse and strain distirbution; elastic deformation; wrinkling; buckling

1. Introduction

Because of the development of advanced nanotechnologies and decreasing dimensions of microelectronic and micromechanical devices, the stability of thin films on substrates subjected to different external loadings becomes an issue of crucial importance. Internal stresses caused by a mismatch in the deformation of the film and the substrate owing to difference in thermal expansion coefficient, elastic modulus, etc. are the driving force of the instability and the development of the surface topography of the films [1]. Periodical wrinkling or random buckling of thin films substantially affecting their physicochemical, mechanical and other properties occurs as a consequence of stress relaxation in the film-substrate system. Buckled surface relief can develop at different scale levels due to film wrinkling under the conditions of viscous flow of the substrate [2], film delamination and buckling [3], progressive cyclic inelastic deformation (ratcheting) [4], etc. Buckling can induce cracking of thin films [3] and subsequent spalling of their pieces leading to the failure of thin-film structures. It was shown that misfit of elastic strains of the film and the substrate causes periodical distribution of normal and tangential stresses at the film-substrate interface [4, 5]. The aim of the work is to demonstrate the universal role of the periodical distribution of stresses and strains at the film-substrate interface underlying the degradation mechanisms of thin films subjected to different external loadings.

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Nomenclature

σ_w	critical wrinkling stress
$\overline{E}_f$	plane-strain modulus of a film
$\overline{E}_s$	plane-strain modulus of a substrate
λ	wrinkle wavelength
σ_b	critical buckling stress
h	film thickness
b	buckling half-width

2. Results and discussion

There are two main buckling modes of thin films on substrates: coherent buckling of the film and the substrate called “wrinkling”, and buckle delamination of the film called “buckling” (see Fig. 1). In the former case, the film should have high adhesive bond with the substrate and not delaminate in the course of the deformation process, while the substrate should be sufficiently compliant to allow coherent deformation with the film. In these circumstances, film instability under the action of applied stresses is extensively governed by the substrate, and when compressive stress exceeds a critical value [6]

$$\sigma_w = \frac{\overline{E}_f}{4}\left(\frac{3\overline{E}_s}{\overline{E}_f}\right)^{2/3}, \tag{1}$$

the film spontaneously buckles resulting in the periodical distribution of wrinkles on its surface (Fig. 1a). These wrinkles each have fixed amplitude/wavelength ratio and relax the stresses by the same value. Depending on the substrate elasticity, wrinkle wavelength and amplitude can be governed by both the energetics and the kinetics of the deformation process. In the case of elastic substrate, wrinkle dimensions are controlled by the minimization of the total elastic energy and determined by the elastic moduli of the film and the substrate, as well as the film thickness. If the substrate is viscous, then wrinkle parameters are governed by only the film characteristics and the stress value.

Wrinkling is clearly revealed after thermal or mechanical loading of elastic metal films deposited on viscoelastic polymer substrates. Fig. 2a shows the wrinkling pattern developed on the surface of the Cu film deposited on the polyimide substrate after annealing at 200 °C. Biaxial compressive stresses due to the difference in coefficients of thermal expansion of the film and the substrate result in wrinkles oriented along perpendicular directions and forming cell structure. Another wrinkling pattern is observed after cooling of thermally grown oxide films on Al alloy substrate. The oxide is elastically deformed, while the metal substrate is subjected to plastic flow by means of creep, resulting in the formation of periodical distribution of crests and valleys on Al_2O_3 film surface (Fig. 2b). Note that the finer wrinkle structure is observed on the surface justifying multilevel character of deformation (Fig. 2c).

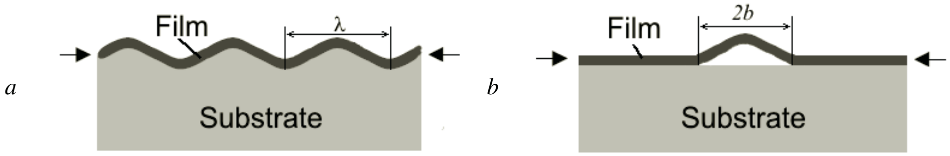

Fig. 1. Buckling modes of thin films on substrates: (a) coherent wrinkling of the film-substrate system; (b) film buckling with delamination along the film-substrate interface

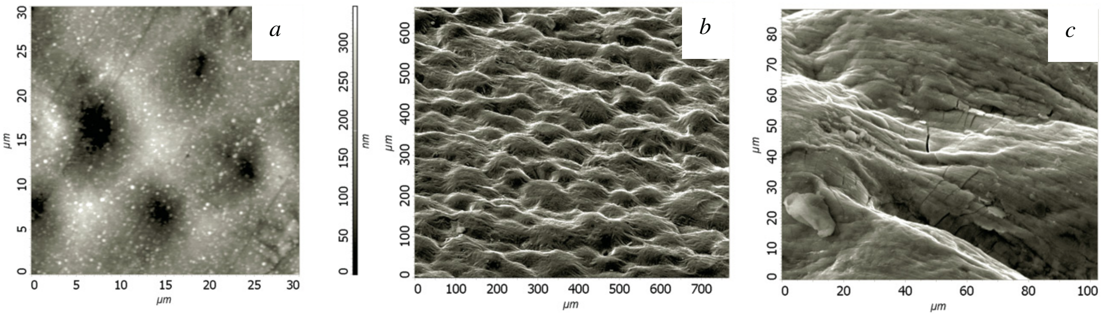

Fig. 2. (a) wrinkling of Cu film on polyimide substrate after annealing at 200 °C (atomic force microscopy); (b, c) wrinkling of oxide film thermally grown at 550 °C on Al alloy (5.6% Mg – 0.4% Mn – 0.32% Sc) substrate (scanning electron microscopy)

A periodical stress distribution develops in the film and at the interface under subsequent compression of the system with wrinkled surface. Fig. 3 shows a schematic illustration of the wrinkles on the film surface and the corresponding stress distribution. Stress component normal to the film-substrate interface varies from a maximum tensile value to zero at the crests and from a maximum compressive value to zero at the valleys [5]. In-plane stresses in the film after wrinkling are also non-uniform [4]. At the crests they are compressive near the film-substrate interface, but can turn into tensile ones close to the free surface after a critical value of wrinkle curvature is exceeded. It testifies that is the bending momentum that tends to increase the wrinkle amplitude. Film cracking can be observed in the boundary regions between crests and valleys of wrinkles, where the normal stresses change sign, i.e. change from tensile into compressive ones (Fig. 2c).

In the case when a film is deposited on a stiff substrate, bending deformation of the film-substrate system is constrained because of the high values of the critical wrinkling stress (Eq. 1). In such circumstances, bonding of the film and the substrate becomes an issue of particular importance. If the bonding is poor or locally weakened by the presence of defects at the interface, the film may partially detach from the substrate. Relaxation of compressive stresses in the detached region of the film results in its buckling, while the substrate stays undeformed. Critical stress for buckling of the detached film area (Fig. 1b) can be written as [1]

$$\sigma_b = \frac{\pi^2}{12}\left(\frac{h}{b}\right)^2 \overline{E}_f . \tag{2}$$

It is seen from Eq. (2) that the critical buckling stress is independent of substrate properties and determined only by elastic properties of the film and *b*/*h* ratio, i.e. the smaller lateral dimensions of the detached film area and the thicker film result in the higher buckling stress.

In spite of the fact that the critical buckling stress is generally independent of the substrate properties, the buckling nature can be substantially governed by the correlation between mechanical characteristics of the film and the substrate. Thus, under the conditions of high adhesion of the film to the substrate and high stress gradients at the film-substrate interface, the buckling pattern is controlled by stress distribution and may be periodical. In this case, initial elastic wrinkling of the film-substrate system is followed by film buckling.

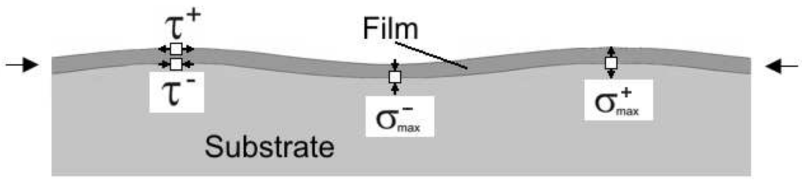

Fig. 3. Distribution of normal (σ) and tangential (τ) stresses in a wrinkled thin film

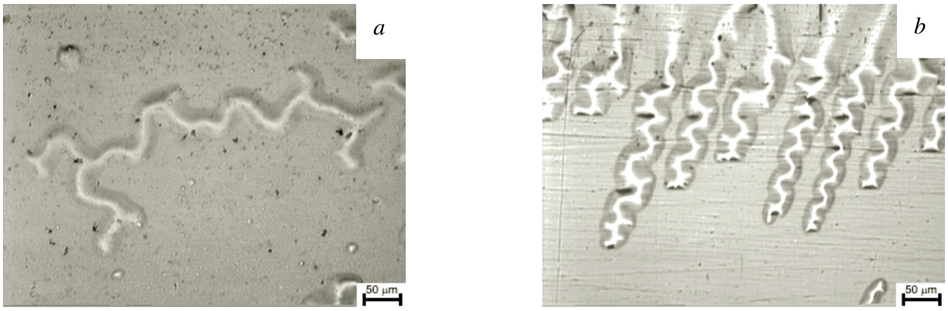

Fig. 4. (a) buckling of Ti film on Ti substrate after 9000 cycles of alternating bending; (b) buckling of Ti film on Al substrate after 200 cycles of alternating bending; (optical microscopy)

Different buckling mechanisms are clearly observed in alternating bending tests of Ti films deposited on Ti and Al substrates. In the case of the Ti/Ti system, first buckles appear only after 1000 cycles of bending. They are randomly distributed on the film surface and have different form and orientation (Fig. 4a). On the contrary, buckling of Ti films on Al substrates starts after a few cycles in the region of maximum bending of the samples. Buckles gradually propagate from the borders of the sample to its center forming a periodical pattern (Fig. 4b).

In the former case, elastic moduli of the film and the substrate are the same and there are no high stress gradients at the interface during bending. Therefore, film delamination is possible only in the regions with poor adhesion, which result from defect accumulation at the film-substrate interface during loading process. In the latter case, considerable difference between elastic moduli of Ti film (120 GPa) and Al substrate (70 GPa) results in high stress gradients at the interface leading to film wrinkling. Detachment of Ti films from the substrate begins at the crests of wrinkles and is due to both normal tensile stresses in these areas and non-uniform substrate strain that leads to the formation of stress concentrators. Film detachment does not result in spalling because the areas with normal tensile stresses are surrounded with areas subjected to normal compressive stresses. The stress-strain state in the neighborhood of a buckled area is highly non-uniform. Compressive stresses relax in the detached area, however, its boundaries are rigidly bonded to the substrate. As a result, high stress gradients develop around the buckled area in the transition zone from the relaxed state to the unrelaxed one. These stress gradients eventually cause the delamination of Ti film by means of interfacial fracture and corresponding change of the form of buckling area.

3. Conclusion

Different kinds of elastic deformation developed in thin films as a result of relaxation of compressive stresses under thermal and mechanical loadings are considered. It is found that the minimization of strain energy in the film-substrate system causes the formation of periodical wrinkles on the film surface. Periodical deformation of the thin film leads to periodical distribution of normal and tangential stresses in the film-substrate system. Depending on the loading conditions, the kinetics of nucleation and accumulation of defects at the film-substrate interface, and the correlation between the properties of the film and the substrate, stress relaxation occurs by means of different mechanisms of elastic film deformation: wrinkling, local buckling, delamination and periodical buckling, etc.

References

1. Freund LB, Suresh S. *Thin film materials: stress, defect formation and surface evolution*. Cambridge: Cambridge university press; 2003.

2. Yoo PJ, Lee HH. Evolution of a stress-driven pattern in thin bilayer films: spinodal wrinkling. *Phys Rev Lett* 2003;**91**: 154502-1-5.

3. Cotterell B, Chen Z. Buckling and cracking of thin films on compliant substrates under compression. *Int J Fract* 2000;**104**:169-179.

4. He MY, Evans AG, Hutchinson JW. The ratcheting of compressed thermally grown thin films on ductile substrates. *Acta Mater* 2000;**48**:2593-2601.

5. Allen HG. *Analysis and design of structural sandwich panels*. New York: Pergamon; 1969.

6. Gong XY, Clarke DR. On the measurement of strain in coatings formed on a wrinkled elastic substrate. *Oxid Met* 1998;**50**:355-376.